Urea, (3-methylphenyl)-

63-99-0 | DTXSID1075351

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.67e-04 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.86e-01

Confidence level: 4.55e-01

Nearest Neighbors from the Training Set

Image not found
Chloroneb
Measured: 5.53e-04
Predicted: 7.69e-03

Image not found
1-Undecene
Measured: 2.46e-03
Predicted: 3.07e-01

Image not found
N-Methylaniline
Measured: 2.60e-02
Predicted: 2.12e-01

Image not found
4-Isopropylphenol
Measured: 1.92e-07
Predicted: 3.08e-02

Image not found
o-Vinyltoluene
Measured: 1.71e-05
Predicted: 1.93